The Claims:

1. (Currently Amended) ~~A system for calculating a potential of mean force (PMF) score of a protein-ligand complex, the system~~ An apparatus comprising:

~~a repulsion term module that:~~

~~accesses one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom pair type of the protein-ligand atom pair;~~

~~using the one or more accessed parameters, calculates the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and~~

~~communicates the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.~~

one or more processors; and

a memory coupled to the processors comprising one or more instructions, the processors operable when executing the instructions to:

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculate a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; and

calculate a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex.

2. (Currently Amended) The system of Claim 1, wherein ~~one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair~~ the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

3. (Canceled)

4. (Canceled)

5. (Currently Amended) The system of ~~Claim 4~~ Claim 2, wherein ~~a set of a plurality of empirically derived minimum binding energy distance and well depth values corresponding to a plurality of protein ligand atom pairs comprises the empirically derived minimum binding energy distance and well depth values corresponding to the atom pair type of the protein ligand atom pair, the set of empirically derived minimum binding energy distance and well depth values yielding a best agreement with a plurality of actual analyzed protein ligand atom pairs~~ a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

6. (Canceled)

7. (Currently Amended) The system of Claim 5, wherein ~~the best agreement between the set of empirically derived minimum binding energy distance and well depth values and the plurality of analyzed protein ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:~~

~~protein ligand complex structures predicted according to the set of empirically derived minimum binding energy distance and well depth values; and~~

~~actual analyzed protein ligand complex structures corresponding to the predicted protein ligand complex structures;~~

root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

8. (Canceled)

9. (Currently Amended) The system of ~~Claim 7~~ Claim 5, wherein one or more of the ~~plurality of sets of empirically-derived minimum binding-energy distance and well-depth values are generated according to one or more of:~~

~~one or more manual processes; and~~

~~one or more automatic processes.~~

first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

10. (Currently Amended) The system of Claim 9, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

11. (Currently Amended) A method ~~for calculating a potential of mean force (PMF) score of a protein-ligand complex, the method~~ comprising:

~~accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;~~

~~using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and~~

~~communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.~~

determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculating a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculating a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; and

calculating a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex.

12. (Currently Amended) The method of Claim 11, wherein ~~one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair~~ the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

13. (Canceled)

14. (Canceled)

15. (Currently Amended) The method of ~~Claim 14~~ Claim 12, wherein ~~a set of a plurality of empirically derived minimum binding-energy distance and well-depth values corresponding to a plurality of protein-ligand atom pairs comprises the empirically derived minimum binding-energy distance and well-depth values corresponding to the atom-pair type of the protein-ligand atom pair, the set of empirically derived minimum binding-energy distance and well-depth values yielding a best agreement with a plurality of actual analyzed protein-ligand atom pairs~~ a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

16. (Canceled)

17. (Currently Amended) The method of Claim 15, wherein ~~the best agreement between the set of empirically derived minimum binding-energy distance and well-depth values and the plurality of analyzed protein-ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:~~

~~protein-ligand complex structures predicted according to the set of empirically derived minimum binding-energy distance and well-depth values; and~~

~~actual analyzed protein-ligand complex structures corresponding to the predicted protein-ligand complex structures.~~

root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

18. (Canceled)

19. (Currently Amended) The method of ~~Claim 17~~ Claim 5, wherein one or more of the ~~plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated according to one or more of:~~

~~one or more manual processes; and~~

~~one or more automatic processes.~~

first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

20. (Currently) The method of Claim 19, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

21. (Currently Amended) ~~Software for calculating a potential of mean force (PMF) score of a protein-ligand complex, the software embodied in computer-readable~~ Logic encoded in one or more media for execution and when executed operable to:

~~access one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;~~

~~using the one or more accessed parameters, calculate the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and~~

~~communicate the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.~~

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

calculate a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; and

calculate a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex.

22. (Currently Amended) The ~~software~~ logic of Claim 21, wherein ~~one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically-derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair.~~ the minimum binding-energy distance value of the atom-pair type is an empirically derived minimum binding-energy distance value of the atom-pair type and the well-depth value of the atom-pair type is an empirically derived well-depth value of the atom-pair type.

23. (Canceled)

24. (Canceled)

25. (Currently Amended) The ~~software~~ logic of ~~Claim 24~~ Claim 22, wherein ~~a set of a plurality of empirically derived minimum binding-energy distance and well-depth values corresponding to a plurality of protein-ligand atom pairs comprises the empirically derived minimum binding-energy distance and well-depth values corresponding to the atom-pair type of the protein-ligand atom pair, the set of empirically derived minimum binding-energy distance and well-depth values yielding a best agreement with a plurality of actual analyzed protein-ligand atom pairs.~~ a first set of empirically derived minimum binding-energy distances and well-depth values comprises the minimum binding-energy distance value and the well-depth value of the atom-pair type, the first set yielding a better agreement with a plurality of actual analyzed protein-ligand atom pairs than one or more second sets of empirically derived minimum binding-energy distances and well-depth values.

26. (Canceled)

27. (Currently Amended) The ~~software~~ logic of Claim 25, wherein ~~the best agreement between the set of empirically derived minimum binding-energy distance and well-depth values and the plurality of analyzed protein-ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:~~

~~protein-ligand complex structures predicted according to the set of empirically derived minimum binding-energy distance and well-depth values; and~~

~~actual analyzed protein-ligand complex structures corresponding to the predicted protein-ligand complex structures.~~

root mean square (RMS) deviation between actual analyzed protein-ligand complex structures and protein-ligand complex structures predicted according to a set of empirically derived minimum binding-energy distances and well-depth values determines agreement between the set of empirically derived minimum binding-energy distances and well-depth values and the actual analyzed protein-ligand atom pairs.

28. (Canceled)

29. (Currently Amended) The ~~software~~ logic of ~~Claim 27~~ Claim 25, wherein one or more of the ~~plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated according to one or more of:~~

~~one or more manual processes; and~~

~~one or more automatic processes.~~

first set of empirically derived minimum binding-energy distances and well-depth values or second sets of empirically derived minimum binding-energy distances and well-depth values are each a product of one or more manual processes or automatic processes.

30. (Currently Amended) The ~~software~~ logic of Claim 29, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

31. (Currently Amended) A system ~~for calculating a potential of mean force (PMF) score of a protein-ligand complex, the system~~ comprising:

~~means for accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;~~

~~means for, using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and~~

~~means for communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.~~

means for determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

means for calculating a repulsion term of the protein-ligand atom pair according to a minimum binding-energy distance value and a well-depth value of the atom-pair type;

means for calculating a potential of mean force (PMF) of the protein-ligand atom pair according to the calculated repulsion term of the protein-ligand atom pair; and

means for calculating a PMF score of the protein-ligand complex according to the calculated PMF of the protein-ligand atom pair, the PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex.